



## Operators and meaning of wave function

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### ABSTRACT

The interpretation problems of quantum theory are considered. In the formalism of quantum theory the possible states of a system are described by a state vector. The state vector, which will be represented as  $|\psi\rangle$  in Dirac notation, is the most general form of the quantum mechanical description. The central problem of the interpretation of quantum theory is to explain the physical significance of the  $|\psi\rangle$ . In this paper we have shown that one of the best way to make of interpretation of wave function is to take the wave function as an operator.

### Indexing terms/Keywords

The state vector; wave function; operators.

### Academic Discipline And Sub-Disciplines

Science; Quantum Physics.

### SUBJECT CLASSIFICATION

Quantum Physics.

### TYPE (METHOD/APPROACH)

Theoretical analysis.

## 1. INTRODUCTION

Quantum theory is the theoretical basis of modern physics that explain behavior of matter on the atomic and subatomic level. Interpretation of quantum theory deals with two problems: how to relate the mathematical formalism of quantum theory to empirical observations, and how to understand that relation terms in ordinary language.

The problem that we have in quantum theory is, what state vector is, or what is a wave function, respectively the measurement process is also analyzed. Interpretation of quantum theory, it is basically an answer to the question what is the state vector, resp. what is a wave function. What is their physical significance? In the Sudbery book [1] the author have indicated at least nine different interpretations used in quantum theory. However, we must say that different interpretations can not be distinguished by purely scientific methods. When the different interpretations give the same experimental results, we have not a different theory.

In this paper we focus our attention on different interpretations in quantum theory mainly how is the meaning of a wave function. Here are not substantially new results, we want to show that the most best acceptable interpretation of the wave function to take it as an operator. We have shown also a relation the probability interpretation with the state vector.

## 2. MEANING OF THE WAVE FUNCTION

When Schrödinger first discovered his equation he discovered the conservation law  $\partial\rho/\partial t = -\nabla\cdot\vec{J}$ , where

$\rho = \psi^*(\vec{r}, t)\psi(\vec{r}, t)$  and  $J$  is "the current density". But he imagined incorrectly that  $\rho$  was the electric current density. It was that Born made an essential contribution, who interpreted the  $\psi$  of the Schrödinger equation in terms of probability amplitude - that the square of the amplitude is not the charge density but is only the probability per unit volume of finding an electron there, and that when you do find electron some place the entire charge is there. The electron is here, or there, or somewhere else, but wherever it is, it is a point charge. Many physicists believe that this interpretation of wave function  $|\psi|^2$  as the density probability is correct.

However, the situation is more complicated. Schrödinger equation is a nonrelativistic equation for particle with spin equals zero. The better equation is relativistic Klein-Gordon equation. But we have the following problem with it. The Klein-Gordon equation has a form as follows



$$\left( \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right) \Phi + \frac{m^2 c^2}{\hbar^2} \Phi = 0. \quad (1)$$

For the Klein-Gordon (KG) equation we can construct  $\rho$ , which is given by the following expression

$$\rho = \frac{i\hbar}{2m} \left( \Phi^* \frac{\partial \Phi}{\partial t} - \Phi \frac{\partial \Phi^*}{\partial t} \right). \quad (2)$$

However, the  $\rho$  we can not make the interpretation of this variable as probability density, because  $\rho$  given by the expression (2) is not positive definite. Since the KG equation is second order,  $\Phi$  and  $\partial \Phi / \partial t$  can be fixed arbitrary at given time, so  $\rho$  make take on negative values, and its interpretation as a probability density have to be abandoned. The interpretation of the KG equation as a single-particle equation, with wave function  $\Phi$ , also has to be abandoned [2].

There is also another problem with the KG equation, and that is the solution  $\frac{E^2}{c^2} - p^2 = m^2 c^2$ , regarded as an equation for  $E$ , is  $E = \pm (m^2 c^4 + p^2 c^2)^{1/2}$ . So solutions of the KG equation contain negative energy terms as well as positive energy ones. Dirac was motivated to find other equation namely the Dirac equation, unlike the KG equation is of first order. It was found that a necessary condition for solution of the Dirac equation exist is  $E = \pm (m^2 c^4 + p^2 c^2)^{1/2}$ . The meaning of the positive energy is clear but that of the negative is not. Schrödinger suggested that a negative energy should be excluded as having no meaning. However, we can not excluded of negative energy states – exist there two reasons [3]. Really, the Dirac equation yields the result that starting with a system in a positive energy state there is a probability of induced transitions into negative energy states. The second objection is mathematical, excluding the negative energy states leads to an incomplete set of wave functions. It is not possible to represent an arbitrary function as an expansion in functions of an incomplete set.

Feynman proposed another interpretation of negative energy states [4]. The idea is that the "negative energy" states represent the states of electron "moving backward in time". However, we can not attach any physical meaning to the „backward running“ process, there are merely a convenient symbolism. Positrons are not electrons running backward in time [5].

The quantum theory of the electromagnetic field is constructed from Maxwell equations by a procedure that is essentially the same as the one that leads to ordinary quantum mechanics. In the quantum mechanics Hamilton classical equations – the  $q_i(t)$  and  $p_i(t)$  – are replaced by operators that satisfy simple rules. In the electromagnetic case, the analogous recipe leads to a reinterpretation of the vector potential  $\vec{A}(\vec{r}, t)$  as a set of operators.

After the Dirac equation was discovered, it was taken that it describes a simple electron, just as Schrodinger equation does. But it soon became clear that the solutions with  $E = \pm (m^2 c^4 + p^2 c^2)^{1/2}$  could not be ignored, nor could they be interpreted as one-electron states. The easiest way to understand the significance of the „negative energy“ solutions is to return to electrodynamics. As we know, photons can be emitted (i.e., created) and absorbed (i.e., destroyed). The quantum procedure leads directly to operators that create and destroy photons. The field operators  $\vec{A}$  is obtained from the classical expression by simply replacing the amplitude by the destruction operator and by creation operator. Creation operator adds a photon to the state while destruction operator removes such a photon. Thus creation operator increases the energy of an arbitrary state by  $\hbar \omega$ , and destruction operator decreases it by  $\hbar \omega$ . This statement provides the correct interpretation of the „negative energies“. After quantization the frequencies that arise from the classical field equations become energy difference, not energies, because the classical field becomes an operator that can both excite and de-excite the state of the field. The "negative energies" are simply energies of deexcitation, and therefore negative. We can make the adequately access to the interpretation of the Dirac equation and its "negative energy" solutions.

We have now discussed two types of quantum field: the scalar and vector field (these things are also valid for the Dirac spinor field). Each of these is an operator function. We know how they are made of certain time-independent creation and annihilation operators: each component  $\theta$  of any of these fields is of the form

$$\theta(x) \equiv \theta(\vec{r}, t) = \int d^3 p \left\{ a(\vec{p}) \exp(-ip \cdot x) + b^+(\vec{p}) \exp(ip \cdot x) \right\}, \quad (3)$$



where  $a(\vec{p})$  is an annihilation operator for a particle, and  $b^+(\vec{p})$  is the creation operator for its antiparticle [1].

The same quantization procedure may also be done for the wave function satisfying Schrödinger equation. This procedure is known as second quantization [6]. Consider a system of  $N$  interacting electrons which move in an external potential. We can divide the Hamiltonian  $H$  of the electronic system into two parts

$$H = \sum_{i=1}^N h(i) + \frac{1}{2} \sum_{i \neq j} v(i, j), \quad (4)$$

where  $h(i)$  is the single-electron operator and  $v(i, j)$  describe the Coulomb repulsion between two electrons  $i$  and  $j$ . Next the Hamiltonian is written in second quantized form, for which we introduce electron field operators  $\psi(\vec{r})$ . They satisfy the following anticommutation relations

$$\{\psi^+(\vec{r}), \psi(\vec{r}')\} = \delta(\vec{r} - \vec{r}'). \quad (5)$$

In terms of them, the Hamiltonian  $H$  takes the form

$$H = \int d^3r \psi^+(\vec{r}) \left( -\frac{1}{2m} \nabla^2 + V(\vec{r}) \right) \psi(\vec{r}) + \frac{1}{2} \int d^3r \int d^3r' \psi^+(\vec{r}) \psi^+(\vec{r}') \frac{1}{|\vec{r} - \vec{r}'|} \psi(\vec{r}') \psi(\vec{r}) \quad (6)$$

In most cases is trying to find approximate eigenstates of  $H$  within a given set of basic functions  $f_j(\vec{r})$ . It is useful to express  $H$  in terms of a given basic set, by associating a set of electron creation and annihilation operators  $a_j^+, a_j$  with the basic. They are obtained through the expansion of the single-electron field operators  $\psi(\vec{r})$  in terms of the  $f_j(\vec{r})$ , i.e.

$$\psi(\vec{r}) = \sum a_i f_i(\vec{r}). \quad (7)$$

The commutation relations for the  $a_j^+, a_j$  follows from those for the  $\psi^+(\vec{r}), \psi(\vec{r})$ . If the overlap matrix reads

$$\int d^3r f_i^*(\vec{r}) f_j(\vec{r}) = \delta_{ij}, \quad (8)$$

the Hamiltonian becomes

$$H = \sum t_{ij} a_i^+ a_j + \frac{1}{2} \sum_{ijkl} V_{ijkl} a_i^+ a_j^+ a_l a_k, \quad (9)$$

where

$$t_{ij} = \int d^3r f_i^*(\vec{r}) \left( -\frac{\hbar^2}{2m} \nabla^2 + V(\vec{r}) \right) f_j(\vec{r}), \quad (10)$$



$$V_{ijkl} = e^2 \int d^3r d^3r' f_i^*(\vec{r}) f_j(\vec{r}) \frac{1}{|\vec{r} - \vec{r}'|} f_k^*(\vec{r}') f_l(\vec{r}'). \quad (11)$$

It means the  $\psi(\vec{r})$ ,  $\psi^+(\vec{r})$  is an operator in nonrelativistic quantum mechanics.

### 3. DISCUSSION AND CONCLUSIONS

In quantum theory possible state of some physical system  $S$  is described by a state vector  $|\psi\rangle$ . To every  $|\psi\rangle$  we ascribe an adjoint vector  $\langle\psi|$  [7]. If  $|\psi\rangle$  and  $|\varphi\rangle$  are two state vectors, their scalar product  $\langle\varphi|\psi\rangle$  is a complex number satisfying  $\langle\varphi|\psi\rangle^* = \langle\psi|\varphi\rangle$ . The quantity  $|\langle\varphi|\psi\rangle|^2$  is the probability that the system will be observed to be in state  $|\varphi\rangle$ , when it is prepared in the state  $|\psi\rangle$ . The scalar product is called the probability amplitude. Any observable quantity associated with the system  $S$ , there corresponds an operator  $A$ . When acting  $A$  on  $|\psi\rangle$ ,  $A$  produced another vector  $A|\psi\rangle$ , and its scalar product with  $\langle\varphi|$ ,  $\langle\varphi|A|\psi\rangle$ , is called a matrix element of  $A$ . It means the state vector can be joined with the probability interpretation of quantum theory.

An interpretation of quantum theory is essentially an answer to the question "What is the state vector, or what is wave function?". Different interpretations cannot be distinguished on scientific grounds. If they do not have different experimental consequences they did constitute different theories. Some other interpretations, and also namely the Transaction interpretation is discussed by Cramer [8]. No one's interpretation is generally accepted.

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